1123-82-406 **Stephen D Levene*** (sdlevene@utdallas.edu), Department of Bioengineering BSB11, University of Texas at Dallas, 800 West Campbell Rd., Richardson, TX 75080-3021, and **Andreas Hanke** (hanke@phys.utrgv.edu), Department of Physics and Astronomy, University of Texas Rio Grande Valley, 80 Fort Brown, Brownsville, TX 78520. *Enhanced understanding of protein-mediated DNA looping, cyclization, and DNA topology through free-energy landscapes.*

Quantitative knowledge of free-energy changes is central to understanding protein and RNA folding, motion and energy transduction in molecular machines, macromolecule-ligand interactions, genome organization, and many other biological phenomena. We consider problems related to DNA tertiary structure and topology, especially loop-mediated interactions involving protein molecules bound to separate sites along DNA. Computing the free-energy cost of forming DNA or chromatin loops entails a delicate and length-scale-dependent balance of enthalpic and entropic contributions and is a challenging problem in statistical mechanics. Moreover, the effects of chromatin organization on such interactions are poorly understood. However, new insights can come from novel experimental approaches along with computational models of DNA flexibility and folding under geometric and/or topological constraints. We have developed a general method for computing free energy landscapes for DNA flexibility and folding across all length scales that is widely applicable to such problems. Applications to protein-mediated topological constraints and enzyme action will be discussed. (Received August 30, 2016)